Non-Linear σ Model for Inhomogeneous Spin Chains

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We derive a non-linear σ model (NLSM) generally representing antiferromagnetic Heisenberg spin chains with inhomogeneous spin magnitudes and inhomogeneous nearest-neighbor exchange constants arrayed in finite periods. Only a restriction is that the average of spin magnitudes on one sublattice is the same as that on the other sublattice. The NLSM gives the gapless condition explicitly written by the spin magnitudes and the exchange constants. We apply this gapless condition to several cases including systems with impurities.

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In 1983 Haldane predicted that an antiferromagnetic Heisenberg spin chain is gapful if the spin magnitude is an integer, and is gapless if it is a half-odd-integer [1]. Since his theory is based on mapping of a spin model to the non-linear σ model (NLSM), the usefulness of the NLSM is recognized by researchers in condensed matter physics. Various interesting aspects of the method of the NLSM are mentioned in some books [2,3,4]. Extension of the NLSM method to systems with inhomogeneity in spins and exchange constants is a challenging problem. It is not only theoretically important but also useful in explaining and suggesting experiments. Affleck reformulated the NLSM method and applied to a spin chain with bond alternation [5]. He divided the spin chain into blocks each of which contains two spins, and defined new variables for each block. Affleck and Haldane analyzed and predicted gapless points for general homogeneous spin chains [6]. Fukui and Kawakami tried to extend the NLSM method to a spin chain including impurities and to spin chains with unit cell containing three and four spins [7,8]. They rather intuitively introduced new variables to form an NLSM and did not care to preserve the degrees of freedom. Hence we cannot determine whether their resultant NLSM's are correct or not by inspecting their theory itself.

In this Letter, we obtain a NLSM generally representing a wide class of inhomogeneous antiferromagnetic spin chains. The derivation is based on the idea dividing the system into blocks [5] but blocks used here are generally defined to contain more than two spins. In a path integral formula, the variables of integration for each block are transformed to form the NLSM with preserving the original degrees of freedom. We apply this NLSM to several cases including systems with impurities and examine gapless conditions.

We consider the spin chain represented by the Hamiltonian

$$H = \sum_{j=1}^{N} J_j \, \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \tag{1}$$

where $\mathbf{S}_j$ is the spin at site j and $J_j(>0)$ is the exchange constant between $\mathbf{S}_j$ and $\mathbf{S}_{j+1}$. The number of lattice sites is N, the lattice spacing is a and the system size is $L = aN$. The quantum number for the magnitude of $\mathbf{S}_j$ is denoted by s_j. The system is periodic with period $2b$ (b: a positive integer):

$$J_{j+2b} = J_j, \quad s_{j+2b} = s_j. \tag{2}$$

We divide the spin chain into blocks each of which contains $2b$ spin sites. The block size $2ba$ is a positive integer (even number) times the size of the unit cell if a unit cell contains an even (odd) number of spins. In a block $\{J_j\}$ and $\{s_j\}$ are arbitrary except for the restriction:

$$\sum_{j=1}^{b} s_{2j} = \sum_{j=1}^{b} s_{2j-1}. \tag{3}$$

This restriction excludes systems with ferrimagnetic ground states in the classical limit.

The partition function Z is written in a path integral formula. When $(-1)^j s_j \mathbf{n}_j$ is the expectation value of $\mathbf{S}_j$ for a coherent state, it is

$$Z = \int D[\mathbf{n}_j] \prod_j \delta(\mathbf{n}_j^2 - 1)\, e^{-S}. \tag{4}$$

The action S at temperature $1/\beta$ is given by

$$S = i \sum_{j=1}^{N} (-1)^j s_j w[\mathbf{n}_j] + \frac{1}{2} \int_0^\beta d\tau \sum_{j=1}^{N} \tilde{J}_j \, (\delta \mathbf{n}_j)^2 \tag{5}$$

with $\delta \mathbf{n}_j = \mathbf{n}_{j+1} - \mathbf{n}_j$ and

$$\tilde{J}_j = J_j s_j s_{j+1}. \tag{6}$$

The first term in Eq. (5) comes from the Berry phase and $w[\mathbf{n}_j]$ is the solid angle which the unit vector $\mathbf{n}_j$ forms in the period β.

We transform spin variables $\{\mathbf{n}_j\}$ into gradually changing variables $\{\mathbf{m}(p)\}$ and small fluctuations $\{\mathbf{L}_q(p)\}$, where p labels a block in the lattice ($p = 1, 2, \cdots, N/2b$) and q labels a site in the block ($q = 1, 2, \cdots, 2b$). The spin variable at the qth site in the pth block is written as

$$\mathbf{n}_{2bp+q} = \Big(1 - \gamma_q \frac{b-q}{2b}\Big)\mathbf{m}(p) + \gamma_q \frac{b-q}{2b}\mathbf{m}(p-\gamma_q) + (-1)^q a \mathbf{L}_q(p), \tag{7}$$

where $\gamma_q = +1(-1)$ for $1 \le q \le b$ ($b+1 \le q \le 2b$). The original constraints $\{\mathbf{n}_j^2 = 1\}$ are changed to $\{\mathbf{m}^2(p) = 1\}$ and $\{\mathbf{m}(p) \cdot \mathbf{L}_q(p) = 0\}$. Here we notice that the number of variables increases in this transformation. To solve the problem we can add an additional constraint for each block which is arbitrary as long as it consists with the other constraints; e. g. $\sum_{q=1}^{2b}(-1)^q \mathbf{L}_q(p) = 0$ or $\mathbf{L}_{2b}(p) = 0$ is a possible one. Hence $2b$ vector variables $\{\mathbf{n}_{2bp+q} | \, q = 1, 2, \cdots, 2b\}$ per block are transformed to $2b$ vector variables $\{\mathbf{m}(p), \mathbf{L}_q(p) | \, q = 1, 2, \cdots, 2b-1\}$ per block; $\mathbf{L}_{2b}(p)$ is written by the other variables through the additional constraint. Also $2b$ original constraints $\{\mathbf{n}_q^2 = 1 | \, q = 1, 2, \cdots, 2b\}$ per block are replaced by $2b$ constraints $\{\mathbf{m}^2(p) = 1, \mathbf{m}(p) \cdot \mathbf{L}_q(p) = 0 | \, q = 1, 2, \cdots, 2b-1\}$ per block. Thus we obtained a new set of variables without changing the original degrees of freedom in the path integral formula (4). In other words, we only transformed the variables of integration. As for the additional constraint, the choice does not affect physical quantities at all. This is because the variables $\{\mathbf{L}_q(p) | \, q = 1, 2, \cdots, 2b\}$ only appear as $\{\mathbf{L}_q(p) + \mathbf{L}_{q+1}(p) | \, q = 1, 2, \cdots, 2b-1\}$ in the partition function, as will be seen.

To take a continuum limit we identify the center of the pth block, $(2bp+b)a$, as coordinate x. Then the difference between adjacent spin variables is replaced as

$$\delta \mathbf{n}_{2bp+q} \to a[\partial_x \mathbf{m}(x) - \mathbf{R}_q(x)] \tag{8}$$

with

$$\mathbf{R}_q(x) = (-1)^q [\mathbf{L}_q(x) + \mathbf{L}_{q+1}(x)]. \tag{9}$$

Equation (9) for $q = 2b$ reads as $\mathbf{R}_{2b}(x) = \mathbf{L}_{2b}(x) + \mathbf{L}_1(x)$. In the Berry phase term of the action (5), the following relation stands due to the restriction (3):

$$\sum_{q=1}^{2b}(-1)^q s_q w[\mathbf{n}_{2bp+q}] = \sum_{q=1}^{2b} \tilde{s}_q \delta w[\mathbf{n}_{2bp+q}], \tag{10}$$

where $\delta w[\mathbf{n}_{2bp+q}] = w[\mathbf{n}_{2bp+q+1}] - w[\mathbf{n}_{2bp+q}]$ and

$$\tilde{s}_q = \sum_{k=1}^{q}(-1)^{k+1} s_k. \tag{11}$$

The continuum limit of the Berry phase term is taken after $\delta w[\mathbf{n}_{2bp+q}]$ is transformed to the τ-integral of $\delta \mathbf{n}_{2bp+q} \cdot (\mathbf{n}_{2bp+q} \times \partial_\tau \mathbf{n}_{2bp+q})$ as in the usual way [3,4]. Thus the action (5) becomes $S_c = S_1 + S_2$ with

$$S_1 = \int_0^\beta d\tau \int_0^L dx \Big\{ -i\frac{s'}{2}(\partial_x \mathbf{m}) \cdot (\mathbf{m} \times \partial_\tau \mathbf{m}) + \frac{a}{2}\bar{J}(\partial_x \mathbf{m})^2 \Big\}, \tag{12}$$

$$S_2 = \int_0^\beta d\tau \int_0^L dx \frac{1}{2b} \sum_{q=1}^{2b} \Big(\frac{a}{2}\tilde{J}_q \mathbf{R}_q^2 + i \mathbf{f}_q \cdot \mathbf{R}_q \Big), \tag{13}$$

where $s' = \sum_{q=1}^{2b} \tilde{s}_q / b$, $\bar{J} = \sum_{q=1}^{2b} \tilde{J}_q / 2b$ and $\mathbf{f}_q = ia\tilde{J}_q(\partial_x \mathbf{m}) + \tilde{s}_q(\mathbf{m} \times \partial_\tau \mathbf{m})$.

The variables $\{\mathbf{L}_q\}$ appear only as $\{\mathbf{R}_q\}$ in the action S_c. The variables $\{\mathbf{R}_q\}$ are not independent and equation $\sum_{q=1}^{2b} \mathbf{R}_q = 0$ stands due to the definition (9); e. g. we can delete $\mathbf{R}_{2b}$ by the equation. We treat the equation as a new constraint. The constraints $\{\mathbf{m} \cdot \mathbf{L}_q = 0\}$ are rewritten as $\{\mathbf{m} \cdot \mathbf{R}_q = 0\}$. Instead of deleting some variables by constraints, we insert the corresponding δ-functions into the path integral formula (4) and treats all the variables independently. We use the integral representations of $\delta(\sum_{q=1}^{2b} \mathbf{R}_q)$ and $\delta(\mathbf{m} \cdot \mathbf{R}_q)$ with integration variables $\mathbf{u}$ and α_q. Then the following term appears in addition to the action S_c:

$$S_3 = \int_0^\beta d\tau \int_0^L dx \frac{i}{2b} \sum_{q=1}^{2b} \mathbf{R}_q \cdot (-\mathbf{u} + \alpha_q \mathbf{m}). \tag{14}$$

Carrying out integrations in the partition function first with respect to $\{\mathbf{R}_q\}$ and then to $\mathbf{u}$, $S_2 + S_3$ reduces to

$$S_2' = \int_0^\beta d\tau \int_0^L dx \frac{1}{4ba} \sum_{q=1}^{2b} \frac{1}{\tilde{J}_q} (\mathbf{F}_q^2 - \bar{\mathbf{F}}^2), \tag{15}$$

where $\mathbf{F}_q = \mathbf{f}_q + \alpha_q \mathbf{m}$ and

$$\bar{\mathbf{F}} = \sum_{q=1}^{2b} (\tilde{J}_q)^{-1} \mathbf{F}_q / \sum_{q=1}^{2b} (\tilde{J}_q)^{-1}. \tag{16}$$

Expanding the integrand in Eq. (15), we find that $\{\alpha_q\}$ appear only in a bilinear form and are integrated out.

Collecting S_1 and the remnant of S_2' after the integration with respect to $\{\alpha_q\}$, we have the final effective action:

$$S_{\text{eff}} = \int_0^\beta d\tau \int_0^L dx \Big\{ -i\frac{J^{(0)}}{J^{(1)}} \mathbf{m} \cdot (\partial_\tau \mathbf{m} \times \partial_x \mathbf{m}) + \frac{1}{2aJ^{(1)}} \Big(\frac{J^{(1)}}{J^{(2)}} - \frac{J^{(0)}}{J^{(1)}} \Big) (\partial_\tau \mathbf{m})^2 + \frac{a}{2} J^{(0)} (\partial_x \mathbf{m})^2 \Big\}, \tag{17}$$

where $\{J^{(n)}\}$ are defined as

$$\frac{1}{J^{(n)}} = \frac{1}{2b}\sum_{q=1}^{2b}\frac{(\tilde{s}_q)^n}{\tilde{J}_q} \quad (n=0,1,2) \tag{18}$$

with Eqs. (6) and (11). Thus we have obtained the action of the NLSM describing the Hamiltonian (1) in the continuum limit. The real-space cutoff is the length of a block of the minimum size. The topological angle θ is given by setting $J^{(0)}/J^{(1)}$ in the first term as $\theta/4\pi$. The velocity v and the coupling constant g are given by equating the coefficients of $(\partial_\tau \mathbf{m})^2$ and of $(\partial_x \mathbf{m})^2$ as $1/2gv$ and $v/2g$ respectively. Note that the coefficient of $(\partial_\tau \mathbf{m})^2$ is always positive.

The action (17) is independent of the way to divide the system into blocks. First we displace each block by one site. Then the spin magnitudes in a new block are ordered as $(s_2, s_3, \cdots, s_{2b}, s_1)$ instead of $(s_1, s_2, s_3, \cdots, s_{2b})$. Denoting quantities related to the new blocks by letters with prime, we have relations $\tilde{s}'_q = s_1 - \tilde{s}_{q+1}$ for $1 \le q \le 2b-1$ and $\tilde{s}'_{2b} = 0$. Using these relations we obtain the following transformation: $J'^{(0)} = J^{(0)}$,

$$\frac{1}{J'^{(1)}} = \frac{s_1}{J^{(0)}} - \frac{1}{J^{(1)}},\ \frac{1}{J'^{(2)}} = \frac{s_1^2}{J^{(0)}} - \frac{2s_1}{J^{(1)}} + \frac{1}{J^{(2)}}. \tag{19}$$

This transformation do not change the coefficient of $(\partial_\tau \mathbf{m})^2$ in Eq. (17). The topological angle (divided by 2π) changes as

$$\frac{2J'^{(0)}}{J'^{(1)}} = 2s_1 - \frac{2J^{(0)}}{J^{(1)}}. \tag{20}$$

Here the first term of $2s_1$ is an integer and does not affect physics. The negative sign of the second term is also irrelevant. Thus the action (17) is invariant under the block displacement.

Second we inspect the effect for the action when we use the block of size $2rba$ (r: a positive integer) instead of $2ba$. The order of the spin magnitudes in a new block is then r times repetition of $(s_1, s_2, \cdots, s_{2b})$. Because of the restriction (3) we have relation $\tilde{s}'_{2jb+q} = \tilde{s}_q$ for $q = 1, 2, \cdots, 2b$ and $j = 1, 2, \cdots, r$. Using this relation we see that $J'^{(n)} = J^{(n)}$ for $n = 0, 1, 2$ and the action (17) is invariant under the block enlargement.

The NLSM has a gapless excitation when $\theta/2\pi$ is a half-odd-integer. This condition is written as

$$\frac{2J^{(0)}}{J^{(1)}} = \frac{2l-1}{2}, \tag{21}$$

where l is an arbitrary integer. In what follows we examine this condition for several cases.

We first apply the general formula (17) to the homogeneous case: $s_1 = s_2 = \cdots = s_N \equiv s$ and $J_1 = J_2 = \cdots = J_N \equiv J$. In this case Eq. (18) gives $J^{(0)} = Js^2$, $J^{(1)} = 2Js$ and $J^{(2)} = 2J$. The coefficients in Eq. (17) are simple as $\theta/4\pi = s/2$, $1/2gv = 1/8aJ$ and $v/2g = aJs^2/2$. Hence Eq. (17) in this case is equivalent to the NLSM which Haldane originally considered [1].

For $b = 1$, a block contains only two spins and the restriction (3) reads as $s_1 = s_2$. Although the correct NLSM in this case has been already obtained [2,5], we restate some results based on the general formula (17). $\{J^{(n)}\}$ are calculated as $J^{(0)} = 2s^2 J_1 J_2/(J_1+J_2)$, $J^{(1)} = 2sJ_1$ and $J^{(2)} = 2J_1$. The gapless condition (21) is then $sJ_2/(J_1+J_2) = (2l-1)/4$. This equation gives the single gapless point $J_2/J_1 = 1 (l=1)$ for $s = 1/2$ and $J_2/J_1 = 1/3 (l=1)$ for $s = 1$. Numerical calculations for $s = 1$ show that the gapless point is at $J_2/J_1 = 0.6$ [9,10] and an experiment for [{Ni(333-tet)(μ-N_3)}$_n$]$(ClO_4)_n$ agrees with this value [11]. Hence the method of the NLSM does not always give quantitatively correct results. However the NLSM is expected to represent the essence of quantum spin systems.

For $b = 2$, the restriction (3) is now $s_1 + s_3 = s_2 + s_4$. In the case of $s_1 = s_2$, $s_3 = s_4$, $J_1 = J_3$ and $J_2 = J_4$, we have $2J^{(0)}/J^{(1)} = 2s_1 s_3 (s_1+s_3)/(s_1^2+s_3^2+2s_1 s_3 J_1/J_2)$. Following the condition (21), a gapless excitation appears at $J_2/J_1 = 4/7$ for $s_1 = 1/2$ and $s_3 = 1$, and at $J_2/J_1 = 3/7$ for $s_1 = 1/2$ and $s_3 = 3/2$. For $s_1 = 1$ and $s_3 = 2$, two gapless points are $J_2/J_1 = 4/19$ and $4/3$. Fukui and Kawakami [8] have obtained the same results [12]. Tonegawa et al. performed numerical calculation for $s_1 = 1/2$ and $s_3 = 1$, and obtained $J_2/J_1 = 0.77 \pm 0.01$ for the gapless point [13]. In the case of $s_1 = s_2$, $s_3 = s_4$, $J_1 = J_2$ and $J_3 = J_4$, we have $2J^{(0)}/J^{(1)} = 2s_1 s_3/(s_1+s_3)$. Hence the gapless excitation appears if and only if $s_1 = s_3$ and the value is a half-odd-integer irrespective of the values of J_1 and J_3. In the case of $s_1 = s_2 = s_3 = s_4 \equiv s$, $J_1 = 1-\delta$, $J_3 = 1+\delta$ and $J_2 = J_4 \equiv J$, we have $2J^{(0)}/J^{(1)} = 2sJ/(J+1-\delta^2)$. Chen and Hida performed numerical calculation for $s = 1/2$ and obtained a phase boundary [14]. The positive-J part of their boundary is close to $\delta = (1-J)^{1/2}$ determined by Eq. (21) with $l = 1$.

Using the block of $b = 3$, we can deal with various systems. Here we examine the case that a unit cell contains three sites. In a block of the minimum size, the spin magnitudes and the exchange constants are ordered as $(s_1, s_2, s_3, s_1, s_2, s_3)$ and $(J_1, J_2, J_3, J_1, J_2, J_3)$. The restriction (3) is satisfied. In this case we have $2J^{(0)}/J^{(1)} = s_1 - s_2 + s_3$ irrespective of the values of J_1, J_2 and J_3. The condition (21) says that systems with one or three half-odd-integer spins in a unit cell are gapless [8,15].

We examine a bond impurity system in the general formula (17). In this system all the spin magnitudes are the same and denoted by s; $\{\tilde{s}_q\}$ are the same as those for the homogeneous case. In contrast there are two kinds of exchange constants, J_0 and J. We assume that $2h$ impurity bonds with J_0 randomly distribute among host bonds with J in a block of size $2b$. Then $(J^{(0)})^{-1}$ is calculated as $[1+\rho_0(J/J_0-1)]/Js^2$ with impurity density $\rho_0 = h/b$; the randomness does not affect this quantity. For $(J^{(1)})^{-1}$ we take an ensemble average since the contribution of an impurity bond changes whether the impu-

rity site q is even or odd. We assume that all the possible distributions occur in the equal probability and that just half of the impurity bonds are on odd sites in the average. Hence we have $(J^{(1)})^{-1} = [1 + \rho_0(J/J_0 - 1)]/2Js$. The topological angle is given by $\theta/2\pi = 2J^{(0)}/J^{(1)} = s$. Therefore the bond impurities do not change the gapless condition of the homogeneous case [16]. Kawae et al. [17] argued that this model stands in the $s = 1$ Haldane system $(CH_3)_4NNi(NO)_3$ (TMNIN) when nonmagnetic impurities Zn^{2+} are doped. They observed spin gaps at some impurity densities.

The last example is a site impurity system where impurity spins are located among host spins. The spin magnitude is s_0 for an impurity spin against s for a host spin. Exchange constants are J_0 for both sides of an impurity site and are J otherwise. The number of impurity spins in a block is $2h$. They are located on the sites of $\{k_j | \, j = 1, 2, \cdots, 2h\}$ in the block. Their distribution is random in the block and the impurity density is $\rho_0 = h/b$. In the calculation of $\tilde{s}_q$ on Eq. (11), we notice that it becomes $\tilde{s}_q^{(0)} \equiv \sum_{k=1}^{q}(-1)^{k+1}s$ for a pure spin system. We now replace the kth term in $\tilde{s}_q^{(0)}$ by $(-1)^{k+1}s_0$ if an impurity spin locates at the kth site. Then we have

$$\tilde{s}_q = \tilde{s}_q^{(0)} + (s - s_0)\sum_{j=1}^{2h}(-1)^{k_j}\theta(q - k_j), \tag{22}$$

where the step function $\theta(x)$ is 1 for $x \geq 0$ and 0 otherwise. Taking the ensemble average with equal weight for all possible distributions, we have

$$\frac{2J^{(0)}}{J^{(1)}} = s\frac{1 + (1 + \frac{s_0}{s})\tilde{\rho}_0}{1 + 2\tilde{\rho}_0} \tag{23}$$

with $\tilde{\rho}_0 = \rho_0(Js/J_0s_0 - 1)$. Derivation of this equation will be reported elsewhere. When $J_0s_0 < Js$, the gapless condition (21) gives the following results. In the case of $s = 1$, Eq. (21) has no integer solution of l for $s_0 \leq 2$. That is, impurities with $s_0 \leq 2$ do not force the gapful excitation of a homogeneous $s = 1$ spin system to be gapless [16,18]. In the case of $s = 1/2$, Eq. (21) has no integer solution of l for $1 \leq s_0 \leq 5/2$.

In summary, we obtained the NLSM (17) for a general antiferromagnetic Heisenberg spin chain with inhomogeneous spin magnitudes and inhomogeneous nearest-neighbor exchange constants arrayed in a finite period. We applied this formula to several cases and examined the gapless conditions. Since the formula is general, it can be applied to various cases which were not treated here. Extensions of the present NLSM method to ladder chains and two or three dimensional systems are future problems.

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[18] Fukui and Kawakami examined a similar spin model but they considered impurity spins at regular intervals [7]. They derived another NLSM from the spin model in a different way. Based on the NLSM they concluded that a gapful system can change to be gapless at some cases.